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Analysis of multitone holographic interference filters by use of a sparse Hill matrix method

Damon W. Diehl and Nicholas George

A theory is presented for the application of Hill's matrix method to the calculation of the reflection and transmission spectra of multitone holographic interference filters in which the permittivity is modulated by a sum of repeating functions of arbitrary period. Such filters are important because they may have two or more independent reflection bands. Guidelines are presented for accurately truncating the Hill matrix, and numerical methods are described for finding the exponential coefficient and the coefficients of the Floquet–Bloch waves within the filter. The latter calculation is performed by use of a computational technique known as inverse iteration. The Hill matrix for such problems is sparse, and thus, even though the matrix can be quite large, it may be efficiently stored and processed by a desktop computer. It is shown that the results of using Hill's matrix method are in close agreement with numerical calculations based on thin-film decomposition, a transfer-matrix technique. An important result of this research is the demonstration that Hill's matrix method may, in principle, be used to analyze any multiperiodic problem, so long as the periods are known to finite precision. © 2004 Optical Society of America

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1. Introduction

Holographic mirrors (also known as pure-reflection holographic gratings) have wavelength selectivity properties and may be thought of as a class of interference filters. This notion of wavelength selectivity may be traced back to some of the earliest experimental work in interferometry.[1–3] For the history of reflection holography, the reader is directed to a publication of collected reprints.[4] Of particular interest are interference filters that reflect at multiple wavelength bands. Such filters have been fabricated by vacuum sputtering[5] and also through holographic processes.[6,7] A comprehensive overview of methods for analyzing reflection of light from films of continuously varying refractive index has been published in the treatise by Jacobsson.[8] Jacobsson discusses a transfer-matrix method in which an inhomogeneous film is modeled as a stack of thin homogeneous layers; that technique is referred to herein as thin-film decomposition. An analogous method for the analysis of volume gratings, called thin-grating decomposition, has been introduced by Alferness[9,10] and further developed by others.[11,12] Although dielectric gratings are not the subject of this paper, we include a few relevant citations that sample some of the key references in this extensive field.[13–19] More central to the topic are those publications that deal specifically with holographic mirrors.[20–22]

In the general study of waves in a periodic structure, one of the more important theoretical approaches depends on Hill's matrix method. This method of solution was discovered by the astronomer G. W. Hill in 1886 and used for the analysis of lunar perigee[23]; it was generalized to wave-propagation problems by Lord Rayleigh in the subsequent year.[24] Excellent treatments of Hill's equation, Floquet's theorem, and Hill's matrix method are presented by Whittaker and Watson[25] and by Magnus and Winkler.[26] Hill's matrix method has been applied to quantum mechanical oscillators by Biswas *et al.*[27] A comprehensive review of the work on electromagnetic waves in periodic structures, which mentions Hill's matrix method, has been published by Elachi.[28] Close agreement has been reported between Hill's matrix method and the extended coupled-waves analysis of Su and Gaylord.[29]

In this paper we demonstrate that Hill's matrix method may be used to analyze the normal-incidence reflection properties of multitone holographic interference filters, where multitone refers to an interference filter designed to reflect two or more wavelength

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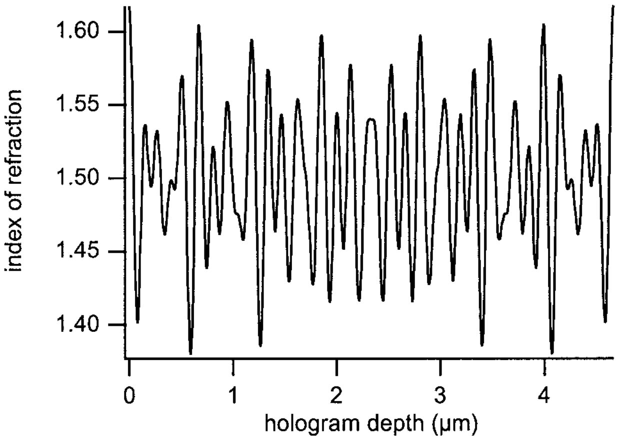

Fig. 1. Index of refraction versus hologram depth for one period of the example problem.

bands. The index profiles for such interference filters comprise the sum of repeating functions of arbitrary period and are generally quite complicated, as is illustrated by Fig. 1, which presents a portion of the index profile of an example three-tone filter, to be further studied in Section 3 below. Such filters were analyzed previously by thin-film decomposition and coupled-wave theory.[30]

In Section 2 it is established that Floquet's theorem may also be applied to a multitone problem, so long as a least common multiple (LCM) can be defined for the periods. In this case the differential equation may be transformed into an infinite system of homogeneous linear equations, which may be written in the form of an infinite matrix (the Hill matrix) multiplied by an infinite vector. This is analogous to an eigenvector problem. To find the solution, we present a procedure for determining the truncation size of the matrix, a numerical technique for finding the exponential coefficient (analogous to an eigenvalue), and a method of inverse iteration to determine the coefficients of the Floquet–Bloch waves within the film (analogous to an eigenvector).

In Section 3 we perform an example calculation, using Hill's matrix method to find the reflection spectrum of a three-tone holographic interference filter. In an independent method of solution, the result from Hill's matrix method is compared with the solution found by use of thin-film decomposition; good agreement is found.

2. Theory

Consider a lossless dielectric medium with a one-dimensional permittivity modulation described by the sum of two or more periodic functions of arbitrary period. This modulation may be described mathematically by the following formula:

$$\epsilon(z) = \sum_{l=1}^{N} f_l(z), \tag{1}$$

where $f_l(z) = f_l(z + \Lambda_l)$. We wish to calculate the reflection and transmission efficiencies for light incident upon this material at normal incidence, propagating in the $\hat{\mathbf{z}}$ direction with the electric field polarized in the $\hat{\mathbf{x}}$ direction. For these calculations it is assumed that the material is linear and isotropic and that the incident plane wave has a harmonic time dependence of $\exp(+i\omega t)$. The amplitude of the electric field, E_x, within the filter may then be described by use of the Helmholtz equation

$$\frac{\partial^2}{\partial z^2} E_x(z) + \frac{{k_0}^2}{\epsilon_0} \epsilon(z) E_x(z) = 0, \tag{2}$$

where ϵ_0 is the permittivity of free space and $k_0 = \omega/c = 2\pi/\lambda$. λ is the free-space wavelength of the incident light.

We wish to apply Floquet's theorem to this problem. Floquet's theorem states that, for any linear differential equation in which all the coefficients have period 2π, a basis for the solutions is $\exp(+\mu\xi)\phi(+\xi)$ and $\exp(-\mu\xi)\phi(-\xi)$, where μ is complex, ξ is a real, unitless variable, and $\phi(\xi)$ is a complex function with period 2π.[25] In this paper, μ is referred to as the exponential coefficient.

Floquet's theorem may be applied to Eq. (2) whenever $\epsilon(z)$ is periodic, so long as the change of variable $\xi = 2\pi z/\Lambda$ is made, where Λ is the period of $\epsilon(z)$. Equation (2) then takes the following form:

$$\left(\frac{2\pi}{\Lambda}\right)^2 \frac{\partial^2}{\partial \xi^2} E_x(\xi) + \frac{{k_0}^2}{\epsilon_0} \epsilon(\xi) E_x(\xi) = 0. \tag{3}$$

This prompts the question: "Under what circumstances will a permittivity profile, as described by Eq. (1), be periodic?" The answer is that the index profile is periodic if and only if there exists a LCM for the periods $\{\Lambda_1, \Lambda_2, \ldots, \Lambda_N\}$. The LCM is defined as the smallest number that is an integer multiple of all of the periods. The periods themselves need not be integers, however. For example, for the numbers 1.2, 1.5, and 2.1, the LCM is 42. A sufficient condition for the existence of the LCM for the set of periods is that each of the periods be known to finite precision. For this paper we assert that such is the case, allowing the use of Floquet's theorem.

Because $\epsilon(\xi)$ is periodic, it may be expanded in a Fourier series. Equation (3) may thus be written as

$$\frac{\partial^2}{\partial \xi^2} E_x(\xi) + \left[\sum_{m=-\infty}^{\infty} \theta_m \exp(im\xi)\right] E_x(\xi) = 0, \tag{4}$$

where a factor of $(\Lambda/2\pi)^2({k_0}^2/\epsilon_0)$ has been absorbed into the summation coefficients, θ_m. Defining ϵ_a to be the permittivity of the film in the limit of no modulation and using the relation $\epsilon = \epsilon_0 n^2$ yield a value of θ_0 given by the formula $\theta_0 = (\Lambda/2\pi)^2(k_0 n_a)^2$, where n_a is the index that corresponds to a permittivity of ϵ_a. Recall that k_0 is wavelength dependent and thus that the θ_m coefficients are also wavelength dependent.

Floquet's theorem assures us that Eq. (4) has a solution of the form

$$E_x(\xi) = \exp(\mu\xi)\phi(\xi) = \exp(\mu\xi) \sum_{l=-\infty}^{\infty} b_l \exp(il\xi), \tag{5}$$

where the periodic function $\phi(\xi)$ has been expanded in a Fourier series. Substituting Eq. (5) into Eq. (4) yields

$$\exp(\mu\xi) \sum_{l=-\infty}^{\infty} \Bigg\{ (\mu + il)^2 b_l \exp(il\xi) + \left[\sum_{m=-\infty}^{\infty} \theta_m \exp(im\xi) \right] b_l \exp(il\xi) \Bigg\} = 0. \tag{6}$$

The b_l terms are the coefficients of the Floquet–Bloch waves within the filter. For Eq. (6) to be valid for all values of ξ, the summation over l must vanish; i.e.,

$$\sum_{l=-\infty}^{\infty} \Bigg\{ (\mu + il)^2 b_l \exp(il\xi) + \left[\sum_{m=-\infty}^{\infty} \theta_m \exp(im\xi) \right] b_l \exp(il\xi) \Bigg\} = 0. \tag{7}$$

Collecting similar powers of $\exp(il\xi)$ yields

$$\sum_{l=-\infty}^{\infty} \exp(il\xi) \left[(\mu + il)^2 b_l + \sum_{m=-\infty}^{\infty} \theta_m b_{l-m} \right] = 0. \tag{8}$$

For Eq. (8) to vanish for all values of ξ, the coefficient of each $\exp(il\xi)$ term must vanish, i.e.,

$$\left[(\mu + il)^2 b_l + \sum_{m=-\infty}^{\infty} \theta_m b_{l-m} \right] = 0 \tag{9}$$

for every integer l.

Dividing by $(l^2 - \theta_0)$ yields the following recursion relation:

$$\frac{(i\mu - l)^2}{l^2 - \theta_0} b_l - \frac{\sum_{m=-\infty}^{\infty} \theta_m b_{l-m}}{l^2 - \theta_0} = 0 \tag{10}$$

for every integer l, which may be written in the form of an infinite matrix multiplied by an infinite vector:

$$\begin{bmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \iddots \\ \cdots & \frac{(i\mu+2)^2 - \theta_0}{2^2 - \theta_0} & \frac{-\theta_1}{2^2 - \theta_0} & \frac{-\theta_2}{2^2 - \theta_0} & \frac{-\theta_3}{2^2 - \theta_0} & \frac{-\theta_4}{2^2 - \theta_0} & \cdots \\ \cdots & \frac{-\theta_{-1}}{1^2 - \theta_0} & \frac{(i\mu+1)^2 - \theta_0}{1^2 - \theta_0} & \frac{-\theta_1}{1^2 - \theta_0} & \frac{-\theta_2}{1^2 - \theta_0} & \frac{-\theta_3}{1^2 - \theta_0} & \cdots \\ \cdots & \frac{-\theta_{-2}}{-\theta_0} & \frac{-\theta_{-1}}{-\theta_0} & \frac{(i\mu)^2 - \theta_0}{-\theta_0} & \frac{-\theta_1}{-\theta_0} & \frac{-\theta_2}{-\theta_0} & \cdots \\ \cdots & \frac{-\theta_{-3}}{1^2 - \theta_0} & \frac{-\theta_{-2}}{1^2 - \theta_0} & \frac{-\theta_{-1}}{1^2 - \theta_0} & \frac{(i\mu-1)^2 - \theta_0}{1^2 - \theta_0} & \frac{-\theta_1}{1^2 - \theta_0} & \cdots \\ \cdots & \frac{-\theta_{-4}}{2^2 - \theta_0} & \frac{-\theta_{-3}}{2^2 - \theta_0} & \frac{-\theta_{-2}}{2^2 - \theta_0} & \frac{-\theta_{-1}}{2^2 - \theta_0} & \frac{(i\mu-2)^2 - \theta_0}{2^2 - \theta_0} & \cdots \\ \iddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ b_{-2} \\ b_{-1} \\ b_0 \\ b_1 \\ b_2 \\ \vdots \end{bmatrix} = 0. \tag{11}$$

The division by $(l^2 - \theta_0)$ in Eq. (10) is necessary to guarantee the convergence of the determinant.[25] Unfortunately, this division introduces singularities into the problem whenever $l^2 - \theta_0 = 0$. Recall that $\theta_0 = (\Lambda/2\pi)^2(k_0 n_a)^2$. Solving for λ, we find that the Hill determinant blows up whenever $\lambda = \Lambda_{\mathrm{LCM}} n_a / l$ for any positive integer l. In solving the problem it is crucial to avoid these singular wavelengths.

The matrix relation in Eq. (11) represents a homogenous system of linear equations. Barring the trivial solution ($b_l = 0$ for every l), the equation can hold only if the determinant of the matrix is identically zero. This determinant is known as Hill's determinant[25] and is indicated by $\Delta(i\mu)$. The value of the exponential coefficient, μ, can be found by solution of the equation $\Delta(i\mu) = 0$. This is analogous to solving the eigenvalue problem $(\mathbf{A} - \mathbf{I}\lambda)\mathbf{v} = 0$, where $\mathbf{A}$ is a square matrix, $\mathbf{I}$ is the identity matrix, λ is an eigenvalue of $\mathbf{A}$, and $\mathbf{v}$ is the eigenvector of $\mathbf{A}$ that corresponds to λ. $(\mathbf{A} - \mathbf{I}\lambda)$ is a function of λ much as the Hill matrix is a function of μ.

Solving the formula $\Delta(i\mu) = 0$ for μ is a daunting undertaking. The task is simplified, however, by the following remarkable relationship:

$$\Delta(i\mu) = \Delta(0) - \frac{\sin^2(\pi i\mu)}{\sin^2(\pi\sqrt{\theta_0})} = 0, \tag{12}$$

where $\Delta(0)$ refers to the determinant of the infinite matrix in the limit $\mu \to 0$. A proof of this relationship is given by Whittaker and Watson.[25]

If the Hill matrix is truncated (as is generally nec-

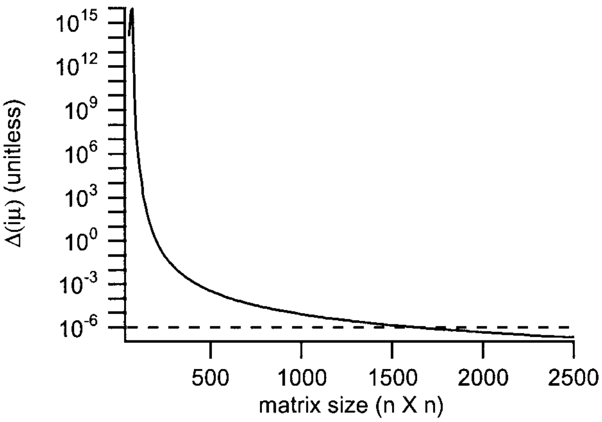

Fig. 2. Value of the Hill determinant, $\Delta(i\mu)$, as a function of matrix size. It can be seen that, as matrix size increases, the values of μ found by solution of Eq. (12) become better approximations of the root of the equation $\Delta(i\mu) = 0$. The dashed line shows that a matrix of 2497×2497 is sufficient to ensure that the Hill determinant is within 10^{-6} of 0. The test wavelength is 350 nm.

essary) the relation in Eq. (12) becomes an approximation. Specifically, a value of μ that makes one side of the equation vanish will not, in general, cause the other side to vanish. Thus a reasonable criterion for truncation is a matrix large enough that the value of μ found by solution of the right-hand side of Eq. (12) causes the Hill determinant on the left-hand side to vanish to within an accepted tolerance. For this paper, a tolerance of 10^{-6} has been chosen. In Fig. 2 the value of the Hill determinant is plotted versus matrix size for a three-tone example problem. The plot shows that, as matrix size increases, the value of μ found by solution of the right-hand side of Eq. (12) becomes a better approximation to the root of the equation $\Delta(i\mu) = 0$. This example is studied further in Section 3 below.

Equation (12) is a transcendental equation with an infinite number of solutions for μ. Each of the solutions is valid, and the solutions will yield identical results once boundary conditions are applied; however, it is most useful to choose the solution that reduces to the proper plane-wave solution in the limiting case of no index modulation. Specifically, when there is no index modulation, a plane-wave solution of the following form is expected:

$$E_x(z) = A \exp(ikz) + B \exp(-ikz), \tag{13}$$

where $k = 2\pi n_a/\lambda$ and λ is the free-space wavelength. Comparing this solution to the form given by Floquet's theorem in Eq. (5) should make clear that Eq. (13) corresponds to the cases when all b_l vanish except for b_0 and when $\mu = \pm i\sqrt{\theta_0}$. In this limiting case, μ is strictly imaginary, and the traveling waves are unattenuated. It is expected that, when the θ_m coefficients are allowed to deviate from zero, μ will develop a small real component at certain resonant wavelengths; however, the imaginary component of μ will remain near the unperturbed value of $\pm i\sqrt{\theta_0}$. This knowledge may be used to pick an initial guess for the value of μ and then to apply Newton's method to search iteratively for the root in that region. Specifically, an initial guess of

$$\mu = \mathrm{Re}\left\{\frac{i}{\pi}\arcsin\left[\sqrt{\Delta(0)}\,\sin(\pi\sqrt{\theta_0})\right]\right\} + i\sqrt{\theta_0} \tag{14}$$

works well.

It is worthwhile to consider under what circumstances the exponential coefficient μ has a real component, as the existence of a real component corresponds to the resonant wavelength bands of the hologram. Studying Eq. (14) reveals that μ has a real component whenever $\arcsin[\sqrt{\Delta(0)}\,\sin(\pi\sqrt{\theta_0})]$ has an imaginary component. It is therefore possible to find the location and width of the expected reflection bands of the film (i.e., the wavelengths for which μ has a real component) without finding the coefficients of the Floquet–Bloch waves or applying boundary conditions.

Once μ has been determined, the next step is to determine the values of the b_n coefficients. This is done by solution of the linear system of equations represented by the matrix relation in Eq. (11). As stated above, it is generally necessary to truncate the matrix to make the problem tractable. For a matrix truncated to a size of $(2m + 1)$ by $(2m + 1)$ (where m is a positive integer), the truncated matrix is denoted $[M_{2m+1}(i\mu)]$, and the system of linear equations becomes

$$[M_{2m+1}(i\mu)]\begin{bmatrix} b_{-m} \\ \vdots \\ b_{-1} \\ b_0 \\ b_1 \\ \vdots \\ b_m \end{bmatrix} = 0. \tag{15}$$

Some subtlety is involved in finding the solution. Because μ has been determined to a finite precision by a numerical method, the Hill determinant $\Delta(i\mu)$ is equal to zero only within the precision limits of the calculation. Because the Hill determinant is not identically zero, standard methods of solving the linear system will result in the trivial solution $b_l = 0$ for every integer l in the range $\{-m, m\}$. To circumvent this obstacle, one may exploit the previously noted similarity between the Hill determinant and an eigenvalue problem. Calculation techniques have been developed for finding the eigenvector of a matrix, given an approximate eigenvalue. Of particular interest is the method of inverse iteration, which is credited to Wilkinson.[31,32] Inverse iteration generates a sequence of normalized vectors $\mathbf{v}_k$ from a given starting vector $\mathbf{v}_0$ by solving the following system of linear equations:

$$(\mathbf{A} - \hat{\lambda}\mathbf{I})\mathbf{v}_k = s_k\mathbf{v}_{k-1}, \qquad k \geq 1, \tag{16}$$

where $\hat{\lambda}$ is an approximation to the eigenvalue λ and s_k is a positive number that is responsible for nor malizing $\mathbf{v}_k$. To perform inverse iteration on the Hill matrix problem we replace $(\mathbf{A} - \hat{\lambda}\mathbf{I})$ in Eq. (16) by the truncated Hill matrix $[M_{2m+1}(i\mu)]$.

It has been demonstrated that a good choice for the initial vector $\mathbf{v}_0$ is a column vector consisting entirely of 1's. Frequently a single iteration yields an eigenvector that has an error less than the uncertainty of the eigenvalue. For an introduction to inverse iteration, the reader is directed to an excellent review paper by Ipsen.[33]

Once this system has been solved for all b_l, one can construct the solution by applying the boundary conditions. Consider a film of thickness L bounded on both sides by homogenous media with a cover index of n_c and a substrate index of n_s. If light with unit amplitude is incident upon the film in the $\hat{\mathbf{z}}$ direction, then the electric field within each of the regions will be of the following form:

$$E_x(z) = \begin{cases} (1)\exp(-ik_0 n_c z) + \rho\exp(+ik_0 n_c z) & z \le 0 \\ \exp\left(-\mu\dfrac{2\pi}{\Lambda}z\right)a^{(-)}\displaystyle\sum_{l=-m}^{m} b_l \exp\left(-il\dfrac{2\pi}{\Lambda}z\right) + \exp\left(+\mu\dfrac{2\pi}{\Lambda}z\right)a^{(+)}\displaystyle\sum_{l=-m}^{m} b_l\exp\left(+il\dfrac{2\pi}{\Lambda}z\right) & 0 \le z \le L, \\ \tau\exp[-ik_0 n_s(z-L)] & z \ge L \end{cases} \tag{17}$$

where ρ and τ are the amplitudes of the reflected and the transmitted waves, respectively, and $a^{(-)}$ and $a^{(+)}$ are the amplitudes for the two Floquet–Bloch solutions within the film. Because the tangential components of the electric and magnetic fields must be continuous across the interfaces at $z = 0$ and $z = L$, the boundary conditions can be expressed by the following four relations:

$$\begin{aligned}
1 + \rho &= a^{(-)}\sum_{l=-m}^{m} b_l + a^{(+)}\sum_{l=-m}^{m} b_l, \\
\tau &= \exp\left(-\mu\frac{2\pi}{\Lambda}L\right)a^{(-)}\sum_{l=-m}^{m} b_l \times \exp\left(-il\frac{2\pi}{\Lambda}L\right) + \exp\left(+\mu\frac{2\pi}{\Lambda}L\right)a^{(+)} \times \sum_{l=-m}^{m} b_l\exp\left(+il\frac{2\pi}{\Lambda}L\right), \\
ik_0 n_c(-1+\rho) &= -a^{(-)}\frac{2\pi}{\Lambda}\sum_{l=-m}^{m} b_l(\mu + il) + a^{(+)}\frac{2\pi}{\Lambda}\sum_{l=-m}^{m} b_l(\mu + il), \\
-ik_0 n_s\tau &= -a^{(-)}\exp\left(-\mu\frac{2\pi}{\Lambda}L\right)\frac{2\pi}{\Lambda}\sum_{l=-m}^{m} b_l(\mu + il)\exp\left(-il\frac{2\pi}{\Lambda}L\right) + a^{(+)}\exp\left(+\mu\frac{2\pi}{\Lambda}L\right)\frac{2\pi}{\Lambda} \times \sum_{l=-m}^{m} b_l(\mu + il)\exp\left(+il\frac{2\pi}{\Lambda}L\right).
\end{aligned} \tag{18}$$

This is a system of four linear equations and four unknowns, which can easily be solved for ρ, τ, $a^{(-)}$, and $a^{(+)}$.

3. Example Calculation with the Hill Matrix Method

Consider a three-tone holographic interference filter with a variation in permittivity described by the equation

$$\epsilon(z) = \epsilon_a + \sum_{j=1}^{3}\epsilon_j\cos\left(\frac{2\pi}{\Lambda_j}z\right) \tag{19}$$

and a thickness of $L = 25\ \mu\text{m}$. We choose $\epsilon_a = 2.25\epsilon_0$ and $\epsilon_1 = \epsilon_2 = \epsilon_3 = 0.1216\epsilon_0$, where ϵ_0 is the permittivity of free space. We wish the filter to reflect the wavelengths $\lambda_1 = 400$ nm, $\lambda_2 = 500$ nm, and $\lambda_3 = 700$ nm when it is illuminated at normal incidence. We expect this to occur when $\Lambda_j = \lambda_j/(2n_a) = \lambda_j/(2\sqrt{\epsilon_a/\epsilon_0})$. Plugging in the appropriate values for λ_j and ϵ_a, we determine that the periods are given by $\Lambda_1 = 133.3300$ nm, $\Lambda_2 = 166.6625$ nm, and $\Lambda_3 = 233.3275$ nm. A plot of the index modulation corresponding to this choice of parameters is shown in Fig. 1. We calculate the reflection spectrum of this multitone holographic interference filter below, using Hill's matrix method and thin-film decomposition.

A. Hill's Matrix Method

A LCM exists for the three periods, and it has the value $\Lambda_{\text{LCM}} = 4.66655\ \mu\text{m}$. Expanding the permittivity in a Fourier expansion, we may determine the

θ_m terms from Eq. (4). Specifically, the values of θ_m are given by the following expression:

$$\theta_m = \left(\frac{\Lambda_{\mathrm{LCM}} k_0}{2\pi}\right)^2 \frac{1}{\epsilon_0} \begin{cases} \epsilon_a & m = 0 \\ \epsilon_3/2 & m = \pm 20 \\ \epsilon_2/2 & m = \pm 28 \\ \epsilon_1/2 & m = \pm 35 \\ 0 & \text{all other } m \end{cases} . \qquad (20)$$

This is enough information to allow us to proceed with constructing the Hill matrix and calculating the Hill determinant. Note that $\theta_m = 0$ for all but seven values of m; thus the matrix comprises mostly zeros. This is known as a sparse matrix. One may greatly economize both computer memory and processing time by keeping track of only the nonzero elements of the matrix. For this reason we used the programming environment Matlab to handle the calculation of the Hill determinant, as it handles sparse matrices well.

As mentioned above, it is not feasible to calculate the determinant of an infinite matrix; therefore a first step toward a solution is truncating the Hill matrix. A reasonable requirement is to find a matrix size such that Eq. (12) is still valid to within an acceptable tolerance. Specifically, a matrix size is desired such that the value of μ found by solution of $\Delta(0) - \sin^2(\pi i\mu)/\sin^2(\pi\sqrt{\theta_0}) = 0$, yields a determinant as close to zero as desired, when μ is substituted into $\Delta(i\mu)$. For a tolerance of 10^{-6}, a matrix size of 2497×2497 is more than sufficient to meet this constraint at the test wavelength, 350 nm, as illustrated in Fig. 2.

Having truncated the matrix, we may solve the equation $\Delta(i\mu) = 0$ for μ by using Newton's method. This must be done for each wavelength to be tested. For this problem the spectrum is calculated over the range 350–750 nm, at a resolution of 0.01 nm. Over this interval singularities will occur near the following wavelengths: 368.412, 388.879, 411.754, 437.489, 466.655, 499.988, 538.448, 583.319, 636.348, and 699.983 nm. Test wavelengths that lie within 0.001 nm of one of these singularities will be skipped. Specifically, the reflection spectrum will not be calculated at 388.88 or 437.49 nm.

Figure 3 is a plot of $\mathrm{Re}(\mu)$ versus free-space wavelength. Similarly, Fig. 4 is a plot of $\mathrm{Im}(\mu)$ versus free-space wavelength. Notice that $\mathrm{Re}(\mu)$ is identically zero except in the vicinity of 400, 500, and 700 nm. These nonzero regions define the reflection bands of the hologram. If finding the reflection bands were our only goal, then the calculation could be stopped here.

Having determined μ, we may use inverse iteration to calculate the 2497-element vector that describes the field structure within the hologram. This exercise must be repeated for every wavelength and the corresponding μ. The individual calculations take only a second or two, but the entire process (with nearly 40,000 wavelengths) takes several hours. However, a lower-resolution spectrum could be calculated in a matter of minutes.

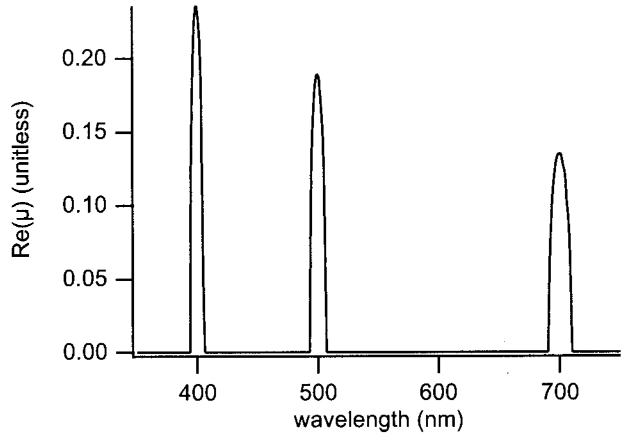

Fig. 3. $\mathrm{Re}(\mu)$ versus free-space wavelength. The regions where $\mathrm{Re}(\mu) > 0$ correspond to the reflection bands of the hologram.

Once the field structure has been determined for each wavelength, the boundary conditions may be applied. These are set out in Eqs. (18). For this problem we have chosen to match the cover and the substrate to the average index of the filter by setting $n_c = n_s = n_a$. Solving for the four unknowns [ρ, τ, $a^{(+)}$, and $a^{(-)}$] is straightforward. Figure 5 is a plot of $R = |\rho|^2$ versus free-space wavelength, as calculated by Hill's matrix method.

B. Thin-Film Decomposition

The accuracy of the above calculation may be confirmed by separate calculations of the reflection spectrum by use of thin-film decomposition. In a previous publication[7] on the fabrication of holographic interference filters, the process of thin-film decomposition was explained in detail. In this sec-

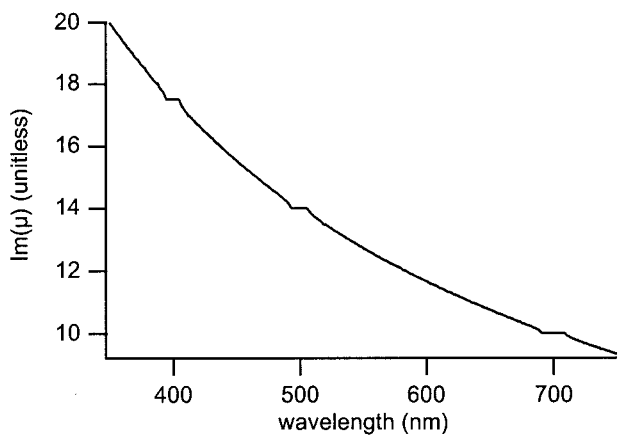

Fig. 4. $\mathrm{Im}(\mu)$ versus free-space wavelength. The flat regions of the curve correspond to the wavelengths for which $\mathrm{Re}(\mu)$ is nonzero.

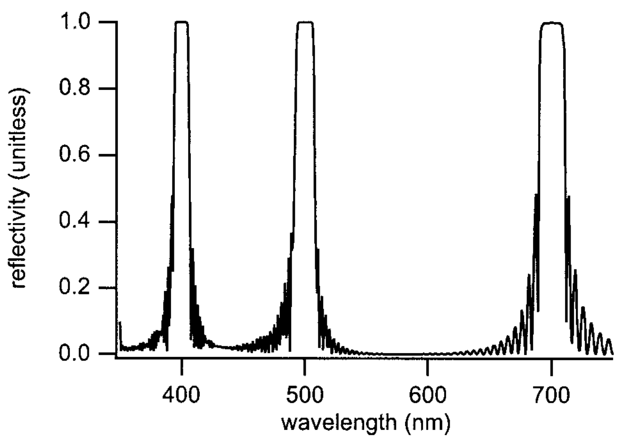

Fig. 5. Reflection spectrum of a three-tone holographic interference filter, as calculated by Hill's matrix technique.

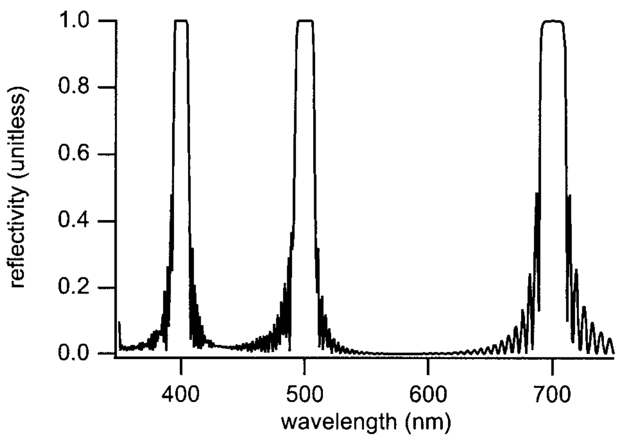

Fig. 6. Reflection spectrum of a three-tone holographic interference filter, as calculated by thin-film decomposition.

tion those results are briefly reviewed and applied to the current problem.

As was previously established,[8] an inhomogeneous stratified medium may be modeled as a stack of thin homogeneous layers. The wave equation can then be solved within each of these homogeneous regions, and one can calculate the reflection and transmission properties of the entire filter by matching the fields at the layer boundaries. The calculations can be expedited by use of matrix notation to characterize each layer. One can then calculate a characteristic matrix for the entire film by chain multiplying the characteristic matrices of each of the decomposition layers. In the research described here, the matrix formalism used by Macleod[34] was used.

It was previously established that, if each period of a holographic interference filter is decomposed into 300 layers, the reflectivity spectrum will be within 10^{-7} of the limiting solution.[35] For the three-tone problem being studied, the smallest period is 133.33 nm, and thus using a layer of 0.44-nm thickness will be more than sufficient to surpass the measurement limits of most spectrophotometers. After the film is decomposed into 56,251 layers, one may then apply transfer-matrix techniques to find the reflection spectrum of the stack of thin films. This spectrum is plotted in Fig. 6 and is clearly quite similar to that plotted in Fig. 5. To compare the two spectra quantitatively, one may calculate the difference between the two, as shown in Fig. 7. The two spectra differ by less than 0.01 (i.e., 1%) over the entire wavelength range.

4. Summary

In this paper a technique has been presented for calculation of the reflection and transmission spectra of multitone holographic interference filters in which the permittivity is modulated by a sum of repeating functions of arbitrary period, as shown in Eq. (1). So long as the component periods are known to finite precision, a least common multiple of the periods will exist, and the filter may be treated as periodic. Floquet's theorem may then be used to posit a solution to the Helmholtz equation. The trial solution is given by Eq. (5). With this trial solution, the Helmholtz equation may be transformed into a recursion relationship for the coefficients of the Floquet–Bloch waves within the material. This recursion relation, given by Eq. (10), may be written as an infinite matrix multiplied by an infinite vector, as shown in Eq. (11). Solving this system of equations is akin to solving an eigenvector problem. Specifically, the exponential coefficient, μ, may be thought of as an eigenvalue of the Hill matrix, and the vector that describes the Floquet-Bloch coefficients may be thought of as the corresponding eigenvector. Determining the exponential coefficient is greatly simplified through the use of the identity given by Eq. (12).

In general, the infinite Hill matrix must be truncated to a finite size. A criterion with which to de-

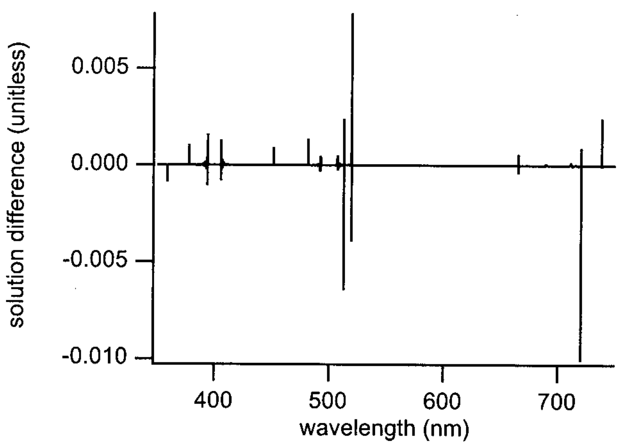

Fig. 7. Difference between the reflection spectra as calculated by Hill's matrix method and by thin-film decomposition. The result of subtracting the thin-film-decomposition spectrum from Hill's matrix method spectrum is shown.

termine how small the matrix may be, while it still yields the desired level of precision, must be found. The criterion presented in this paper is that the identity in Eq. (12) must hold to within a desired level of precision for the truncated matrix.

Equation (12) is a transcendental equation with an infinite number of solutions. Newton's method may be used to solve the equation for μ. Equation (14) is proposed as a good initial guess for μ, as it will converge properly in the limit of zero index modulation.

Once the matrix has been truncated and μ has been determined, the coefficients of the Floquet–Bloch waves within the material must be determined. This is a difficult problem to solve because the value for μ is an approximation, as it has been determined by a numerical method; this can force a trivial solution. We have shown, however, that a solution can be found by use of a technique called inverse iteration.

Given the coefficients of the Floquet–Bloch waves, one finds the solution for a given problem by matching boundary conditions. For a finite multitone structure bounded by semi-infinite homogenous media and illuminated at normal incidence, the appropriate boundary conditions are given by Eqs. (18).

As an example of this technique, a three-tone holographic interference filter was analyzed. Its permittivity is described by Eq. (19) and plotted in Fig. 1. It was determined that a matrix size of 2497×2497 was sufficient for the desired level of precision. The real and imaginary components of exponential coefficient μ are plotted in Figs. 3 and 4. The regions where μ takes on a real component correspond to the reflection bands of the filter. The reflection spectrum of the filter as calculated by Hill's matrix method is plotted in Fig. 5. Excellent agreement was found with the spectrum as calculated by thin-film decomposition, which is plotted in Fig. 6. It is believed that both methods converge to the same solution in their respective limits. The value of using Hill's matrix method is that it provides a closed-form solution for a rather complicated problem. Furthermore, for the example presented here, Hill's matrix method of solution takes ~30% less time than the thin-film decomposition solution; the two yield nearly identical spectra. However, it must be noted that thin-film decomposition is easier to apply to a broader class of problems, particularly when it cannot be argued that the modulation of the permittivity is periodic.

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References

1. O. Wiener, "Stehende Lichtwellen und die Schwingungrichtung polarisirten Lichtes," Ann. Phys. Chem. **40,** 203–243 (1890).
2. G. Lippmann, "Sur la théorie de la photographie des coulars simples et compusées par la méthode interférentielle," J. Phys. (Paris) **3,** 97–107 (1894).
3. P. Connes, "Silver salts and standing waves: the history of interference colour photography," J. Opt. (Paris) **18,** 147–166 (1987).
4. T. W. Stone and B. J. Thompson, eds., *Selected Papers on Holographic and Diffractive Lenses and Mirrors*, Vol. MS 34 of SPIE Milestones Series (SPIE Optical Engineering Press, Bellingham, Wash., 1991).
5. J. B. Adolph, R. W. Bertram, K. L. Yan, P. Zhou, and R. de Leon, "Design and fabrication of multi-line inhomogeneous rejection filters," in *Inhomogeneous and Quasi-Inhomogeneous Optical Coatings*, J. A. Dobrowolski and P. G. Verly, eds., Proc. SPIE **2046,** 141–146 (1993).
6. K. W. Steijn, "Multicolor holographic recording in DuPont holographic recording film: determination of exposure conditions for color balance," in *Holographic Materials II*, T. J. Trout, ed., Proc. SPIE **2688,** 123–134 (1996).
7. D. W. Diehl and N. George, "Holographic interference filters for infrared communications," Appl. Opt. **42,** 1203–1210 (2003).
8. R. Jacobsson, "Light reflection from films of continuously varying refractive index," in *Progress in Optics*, E. Wolf, ed. (North-Holland, Amsterdam, 1966), Vol. 5, Chap. 5, pp. 247–286.
9. R. Alferness, "Analysis of optical propagation in thick holographic gratings," Appl. Phys. **7,** 29–33 (1975).
10. R. Alferness, "Analysis of propagation at the second-order Bragg angle of a thick holographic grating," J. Opt. Soc. Am. **66,** 353–362 (1976).
11. T. W. Stone and N. George, "Wavelength performance of holographic optical elements," Appl. Opt. **24,** 3797–3810 (1985).
12. T. W. Stone, "Holographic optical elements," Ph.D. dissertation (University of Rochester, Rochester, N.Y., 1986).
13. C. V. Raman and N. S. N. Nath, "The diffraction of waves by high frequency sound waves. I, II," Proc. Ind. Acad. Sci. **2,** 406–420 (1935).
14. C. V. Raman and N. S. N. Nath, "The diffraction of waves by high frequency sound waves. III, IV," Proc. Ind. Acad. Sci. **3,** 75–84, 119–125 (1936).
15. H. Kogelnik, "Coupled wave theory for thick hologram gratings," Bell Syst. Tech. J. **48,** 2909–2947 (1969).
16. M. Chang and N. George, "Holographic dielectric grating: theory and practice," Appl. Opt. **9,** 713–719 (1970).
17. M. G. Moharam and T. K. Gaylord, "Rigorous coupled-wave analysis of planar-grating diffraction," J. Opt. Soc. Am. **71,** 811–818 (1981).
18. M. G. Moharam and T. K. Gaylord, "Planar dielectric grating diffraction theory," Appl. Phys. B **28,** 1–14 (1982).
19. P. St. J. Russell, "Optics of Floquet–Block waves in dielectric gratings," Appl. Phys. B **39,** 231–246 (1986).
20. M. G. Moharam and T. K. Gaylord, "Chain-matrix analysis of arbitrary-thickness dielectric reflection gratings," J. Opt. Soc. Am. **72,** 187–190 (1982).
21. Z. Zylberberg and E. Marom, "Rigorous coupled-wave analysis of pure reflection gratings," J. Opt. Soc. Am. **73,** 392–398 (1983).
22. M. G. Moharam and T. K. Gaylord, "Comments on analyses of reflection gratings," J. Opt. Soc. Am. **73,** 399–401 (1983).
23. G. W. Hill, "On the part of the motion of the lunar perigee which is a function of the mean motions of the Sun and Moon," Acta Math. **8,** 1–36 (1886).
24. Lord Rayleigh, "On the maintenance of vibrations by forces of double frequency, and on the propagation of waves through a medium endowed with a periodic structure," Phil. Mag. J. Sci. **24,** 145–159 (1887).
25. E. T. Whittaker and G. N. Watson, *A Course of Modern Anal-*

ysis, 4th ed. (Cambridge U. Press, Cambridge, 1927), Chap. 19, pp. 412–417.

26. W. Magnus and S. Winkler, "Hill's equation," in *Interscience Tracts in Pure and Applied Mathematics*, L. Bers, R. Courant,and J. J. Stoker, eds. (Wiley Interscience, New York, 1966), Vol. 20, Chap. 1, pp. 3–10.
27. S. N. Biswas, K. Datta, R. P. Saxena, P. K. Srivastava, and V. S. Varma, "The Hill determinant: an application to the anharmonic oscillator," Phys. Rev. D **4,** 3617–3620 (1971).
28. C. Elachi, "Waves in active and passive periodic structures: a review," Proc. IEEE **64,** 1666–1698 (1976).
29. D. L. Jaggard and C. Elachi, "Floquet and coupled-wave analysis of higher-order Bragg coupling in a periodic medium," J. Opt. Soc. Am. **66,** 674–682 (1976).
30. X. Ning, "Analysis of multiplexed-reflection holographic gratings," J. Opt. Soc. Am. A **7,** 1436–1440 (1990).
31. J. H. Wilkinson, "The calculation of eigenvectors of codiagonal matrices," Comput. J. **1,** 90–96 (1958).
32. J. H. Wilkinson, "Inverse iteration in theory and practice," in *Symposium Mathematica* (Instituto Nazionale de Alta Matematica, Rome, 1972), Vol. X, pp. 361–379.
33. I. C. F. Ipsen, "Computing an eigenvector with inverse iteration," Soc. Indust. Appl. Math. Rev. **39,** 254–291 (1997).
34. H. A. Macleod, *Thin-Film Optical Filters*, 2nd ed. (McGraw-Hill, New York, 1989).
35. P. Sharlandjiev and T. Mateeva, "Normal incidence holographic mirrors by the characteristic matrix method. Numerical examples," J. Opt. (Paris) **16,** 185–189 (1985).